New parameters (N³) and Formelherstellung (8/17/09)

The state equation stays the same:

$$\frac{dC_{iv}^{j}}{dt} = k_{fi}k_{fadj} \left[C_{im}^{j} \right] S_{v} - k_{bi} \cdot k_{badj} \cdot C_{iv}^{j}$$

forward.

Unsaturation forward:

$$unf = 2^{stdev(un_v)}$$

Charge Forward

$$ch_f = 50^{-\left|\overline{ch_v}\cdot ch_m\right|}$$

Curvature Forward

$$cu_f = 10^{stdev(|\log(cu_v)|)}$$

Length Forward

$$l_f = 3^{stdev(l_v)}$$

Complex Formation 1 (CF1; formerly umbrella)

$$CF1_f = 1$$

 $k_{fadj} = unf \cdot ch_f \cdot cu_f \cdot l_f \cdot CF1_f$

backward:

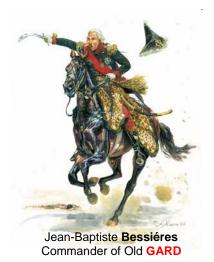
unsaturation backward:

$$unb = 10^{|3.5^{-\overline{un_v}}-3.5^{-un_m}|}$$

Charge backward:

$$chb = 50^{-|\overline{ch_v} \cdot ch_m|}$$

Curvature backward



$$cub = 10^{\left\|cuv - 1\right\| - \left\|cuw - 1\right\|}$$

Length backward

$$lb = 3.2^{\left|\overline{l}_v - l_m\right|}$$

Complex Formation 1 (CF1) backward

$$CF1_b = 1.5^{(CF1_v \cdot CF1_m - |CF1_v \cdot CF1_m|)}$$

 $k_{badj} = unb \cdot chb \cdot cub \cdot lb \cdot CF1_b$

The starting parameters $(k_f = M^{-1}s^{-1}; k_b=s^{-1})$

 $\begin{array}{lll} PC: & k_f = 3.7 \times 10^6 \,; & k_b = 2 \times 10^{\text{-5}} \\ PE: & k_f = 2.3 \times 10^6 \,; & k_b = 1 \times 10^{\text{-5}} \\ PS: & k_f = 3.7 \times 10^6 \,; & k_b = 1.25 \times 10^{\text{-5}} \\ SM: & k_f = 3.7 \times 10^6 \,; & k_b = 3.1 \times 10^{\text{-3}} \,\text{s}^{\text{-1}} \\ CHOL: & k_f = 5 \times 10^8 \,; & k_b = 2.8 \times 10^{\text{-4}} \end{array}$

k_f(PC) taken from Nichols85; weakness: NBD-PC; no unlabeled k+ found.

k_f(PE) taken from Abreu04; NBD-PE

 $k_f(PS)$ and $k_f(SM)$ assumed same as $k_f(PC)$

 $k_f(CHOL)$ is weak – basically guessed from $k_f(NBD-lysoPE)$ in Sampaio05 and $k_f(PC)$; try adjustments, probably decrease

k_b(PC) is taken from Wimley90 − radioactive label; LUV, 30° C.

Then, Nichols82 with C6-NBD-PC and other headgroups was used to determine *ratios* of $k_b(PC)$ with other headgroups, and k_b for other headgroups assigned accordingly. $k_b(PS)$ was assumed to be the same as $k_b(PG)$ given by Nichols82 (also ratio from $k_b(PC)$).

 $k_b(SM)$ is taken from $k_b(PC)$ of Wimley90 (radioactive), and then a ratio of $k_b(PC)/k_b(SM)$ taken from Bai97: = 34/2.2 = 15.45; 2.0 x 10⁻⁴ x 15.45 = 3.1 x 10⁻³ s⁻¹.

k_b(CHOL) taken from Jones90 (radioactive; POPC LUV; 37°).

Curvature:

$$PE = 0.8$$
; $CHOL = 0.8$

Charge:

$$PS = -1$$

CF1

SM = 3; PC = 2; CHOL = -1

Initial concentrations:

1 x 10^{-10} M; gamma distributed with stdev = 10^{-10}